Glenn T. Seaborg Center Seminar

Actinide Metal Atom (Th and U) Reactions to Form Novel Molecules

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Wednesday, Jun 24, 2008
4:00 - 5:00 pm
Building 70A, Room 3377

Reactions of early actinide metal atoms (Th and U) with small molecules to form actinide-carbon multiple bonds will be presented. Matrix infrared spectra and frequency calculations using density functional theory lead to the identification of new actinide methylidene and methylidyne molecules. Although Th is more reactive with methane than U, the $CH_2{=}AnH_2$ molecules have the same 1.92 double bond orders. The $HC{\div}ThF_3$ molecule contains a weak electron-deficient triple bond whereas $HC{\equiv}UF_3$ has a triple bond of 2.56 bond order. The isoelectronic $N{\equiv}UF_3$ molecule contains the strongest triple bond to uranium in a terniary complex, bond order 2.78, yet prepared.

References

1. L. Andrews and H.-G. Cho, "Infrared Spectrum and Structure of $CH_2{=}ThH_2$", *J. Phys. Chem. A* **2005**, *109*, 6796-6798.
2. J. T. Lyon, L. Andrews, P.-Å. Malmqvist, B. O. Roos, T. Yang and B. E. Bursten, "Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, $CH_2{=}UH_2$," *Inorg. Chem.* **2007**, *46*, 4917-4925.
3. J. T. Lyon, L. Andrews, H.-S. Hu, J. Li, "Formation of Unprecedented Actinide≡Carbon Triple Bonds in Uranium Methylidyne Molecules," *Proc. Nat'l. Acad. Sci.* **2007**, 104, 18919-18924.
4. J. T. Lyon and L. Andrews, "Reactions of Thorium Atoms with Polyhalomethanes: Infrared Spectra of the $CH_2{=}ThX_2$, $HC{\div}ThX_3$, and $XC{\div}ThX_3$ Molecules," *Eur. J. Inorg. Chem.* **2008**, 1047-1058.

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